Height correlation of rippled graphene and Lundeberg-Folk formula for magnetoresistance

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(Dated: 9 November 2012)

Abstract

Application of an in-plane magnetic field to rippled graphene will make the system be a plane with randomly distributed vector potentials. Massless Dirac fermions carrying charges on graphene are scattered by the vector potentials and magnetoresistance is induced proportional to the square of amplitude of in-plane magnetic field B_{\parallel}^2 . Recently, Lundeberg and Folk proposed a formula showing dependence of the magnetoresistance on carrier density, in which the coefficient of B_{\parallel}^2 is given by a functional of the height-correlation function c(r) of ripples. In the present paper, we give exact and explicit expressions of the coefficient for the two cases such that c(r) is (i) exponential and (ii) Gaussian. The results are given using well-known special functions. Application of the present solutions in the vicinity of charge neutrality point should be careful because of the possible strong density inhomogeneity in rippled graphene. Here our analytic expressions are proposed, however, as trial interpolation formulas connecting the positive high-carrier-density regime and the negative one for magnetoresistance. Numerical fitting of our solutions to experimental data were performed. It is shown that the experimental data are well-described by the formula for the Gaussian height-correlation of ripples in the whole region of carrier density. The standard deviation Z of ripple height and the correlation length R of ripples are evaluated, which can be compared with direct experimental measurements.

PACS numbers: 72.80.Vp, 05.40.-a, 05.60.-k, 02.30.Gp

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I. INTRODUCTION AND MAIN RESULTS

Graphene, a one-atom-thick allotrope of carbon [1, 2], has attracted much attention of theoretical physicists, since its electronic excitations are described by two-dimensional (2D) massless Dirac fermion (see, for instance, [3, 4]). Let $v_{\rm F}$ be the Fermi velocity. Then, for a free fermion, the 2D massless Dirac equation is given by

$$-i\hbar v_{\rm F} \begin{pmatrix} 0 & \partial_x - i\partial_y \\ \partial_x + i\partial_y & 0 \end{pmatrix} \psi(\mathbf{r}) = E\psi(\mathbf{r}), \tag{1}$$

where $i = \sqrt{-1}$, $\partial_x = \partial/\partial x$, $\partial_y = \partial/\partial y$, and $\psi(\mathbf{r})$ is a two-component wave function with the particle position $\mathbf{r} = (x, y)$. For a wave-number vector $\mathbf{k} = (k_x, k_y)$, the eigenvalues of energy are given by $E = E_{\pm} = \pm \hbar v_{\rm F} k$, $k = |\mathbf{k}|$, where the \pm signs correspond to two values of the helicity of fermion $\hat{h} = \pm 1/2$. The wave functions are determined as [3]

$$\psi_{\pm}(\mathbf{r}; \mathbf{k}) = \langle \mathbf{r} | \mathbf{k} \rangle = \frac{1}{\sqrt{2V}} e^{i\mathbf{k}\cdot\mathbf{r}} \begin{pmatrix} e^{-i\theta_k/2} \\ \pm e^{i\theta_k/2} \end{pmatrix}, \tag{2}$$

where V is the volume of the system and

$$\theta_k = \arctan\left(\frac{k_y}{k_x}\right). \tag{3}$$

Although the basic description of the system is very simple as shown above, physics of graphene is extremely rich, since the 2D Dirac equation is much modified by external electric and magnetic fields applied to the graphene plane as well as by changing geometric and topological features of the 2D surface [3, 4]. As a matter of fact, an ultrathin membrane is unstable in the 3D real space and in suspended graphene and in graphene placed on a substrate nanometer-scale corrugations, which are simply called *ripples* [5], are observed [6–12]. Since spatial distribution of such microscopic structures on the surface cannot be controlled, even when we apply uniform electric and/or magnetic fields, the rippled graphene will behave as a 2D system with randomly distributed scalar and vector potentials on it. Effect of ripples on electronic transport on graphene is an interesting subject both from theory and experiment [3, 4, 13–16].

Recently, magnetotransport measurements on rippled graphene have been reported, where a magnetic field is applied parallel to the averaged 2D plane of the graphene [17–20] (see also [21] for bilayer graphene). If the surface is a perfect plane, such an in-plane

magnetic field \mathbf{B}_{\parallel} does not affect any motion of 2D electron, since electronic motion couples only to the component of magnetic field normal to the 2D plane. But on real graphene, the magnetic field becomes to include a component normal to the surface depending on the local slope around ripples. Then the system has inhomogeneous out-of-plane magnetic fields. With respect to electromagnetic property, we will be able to regard the rippled graphene with \mathbf{B}_{\parallel} as a system of traveling 2D massless Dirac fermions, which are randomly scattered by ripples [4, 17].

In the present paper, we study a formula of Lundeberg and Folk for the magnetoresistance $\Delta \rho$, which was derived from a model based on the Boltzmann transport theory [17, 18]. The relative height of ripple on the averaged 2D plane is denoted by $h(\mathbf{r})$ for each 2D position $\mathbf{r} = (x, y)$. We characterize the height distribution by the two-point height correlation

$$c(\mathbf{r}; \mathbf{r}_0) = \langle h(\mathbf{r}_0)h(\mathbf{r}_0 + \mathbf{r})\rangle, \tag{4}$$

which is defined as a statistical average of product of the height at \mathbf{r}_0 and that at the position separated from \mathbf{r}_0 by a displacement vector \mathbf{r} . For simplicity, we assume that the distribution of $h(\mathbf{r})$ is translation invariant and isotropic in this paper. By this assumptions, (4) becomes independent of \mathbf{r}_0 and it depends only on the distance of two points $r = |\mathbf{r}|$; $c(\mathbf{r}; \mathbf{r}_0) = c(r)$. As a function of wave-number $k = |\mathbf{k}|$ of fermion, we define

$$g(k) = \int_0^\infty rW(rk)c(r)dr,\tag{5}$$

where

$$W(z) = \int_0^{2\pi} J_0\left(2z\sin\frac{\phi}{2}\right)\sin^2\frac{\phi}{2}d\phi\tag{6}$$

with the Bessel function $J_0(z)$ (see Appendix A for special functions [22]). The signed carrier-density of graphene is denoted by $n = n_+ - n_-$, which is the difference of the density of electrons n_+ and that of holes n_- . We assume that the temperature is low and the state is degenerated so that the wave-number of fermion k is well-approximated by the Fermi wave-number $k_{\rm F}$. With counting contributions from the two Dirac points K and K' and spin, $k \simeq k_{\rm F}$ is related with n as (see, for instance, Sect. II.A in [3]),

$$k = k(n) = \sqrt{\pi |n|},\tag{7}$$

where the absolute value of n is used by the particle-hole symmetry; $E_{\pm} = \pm \hbar v_{\rm F} k$. Let $B_{\parallel} = |\mathbf{B}_{\parallel}|$ and θ be the angle between \mathbf{B}_{\parallel} and the direction of the current \mathbf{J} along which

the resistance ρ is measured. Set $\Delta \rho = \rho(B_{\parallel}) - \rho(0)$, the $\boldsymbol{B}_{\parallel}$ -induced part of resistance, which we call magnetoresistance. Then the Lundeberg-Folk formula is given as

$$\Delta \rho(n, \theta, B_{\parallel}) = \frac{\pi B_{\parallel}^2}{2\hbar} (\sin^2 \theta + 3\cos^2 \theta) g(k(n)). \tag{8}$$

Remark that this formula is not given in the published paper [17] of Lundeberg and Folk, but the corresponding equations are found in Appendix of its arXiv version [18]. Lundeberg and Folk introduced a correlation length R > 0 for ripple-height correlation c(r) and argued the asymptotic behavior of g(k) in $k \ll 1/R$ and $k \gg 1/R$, and from the latter estimate the behavior of (8) in high carrier-density region was predicted as $\Delta \rho \sim |n|^{-3/2}$, $|n| \gg 1$. This $|n|^{-3/2}$ -law was emphasized in their paper and has been used for analyzing experimental data [17, 19, 20], while it is an asymptotic law in $|n| \gg 1$ for a special case with the Gaussian height-correlation of ripples as clarified below in the present paper. Here we call the general equation (8) the Lundeberg-Folk formula.

The main purpose of the present paper is to show that, for the two cases

(i)
$$c(r) = Z^2 e^{-r/R}$$
 (exponential), and

(ii)
$$c(r) = Z^2 e^{-(r/R)^2}$$
 (Gaussian),

with a variance of height $Z^2 = c(0) = \langle h(\mathbf{r}_0)^2 \rangle = \langle h^2 \rangle$, exact and explicit representations for the anisotropic magnetoresistance (8) are obtained. (For the Gaussian correlated disorder, see [23].) The results are the following. Let $F(\alpha, \beta, \gamma; z)$ and $F(\alpha, \gamma; z)$ be the Gauss hypergeometric function and the confluent hypergeometric function, respectively (see Appendix A for definitions and basic properties of special functions used in this paper). Then, for (i) the exponential height-correlation

$$g(k) = \pi (ZR)^2 F\left(\frac{3}{2}, \frac{3}{2}, 2; -(2kR)^2\right)$$
$$= \frac{Z^2}{k^2} \left[K(2ikR) - \frac{1}{1 + (2kR)^2} E(2ikR) \right], \tag{9}$$

and for (ii) the Gaussian height-correlation

$$g(k) = \frac{\pi Z^2 R^2}{2} F\left(\frac{3}{2}, 2; -(kR)^2\right)$$

$$= \frac{\pi (ZR)^2}{2} \left[I_0((kR)^2/2) - I_1((kR)^2/2) \right] e^{-(kR)^2/2}, \tag{10}$$

where K(z) (resp. E(z)) is the complete elliptic integral of the first (resp. of the second) kind, and $I_{\nu}(z)$ is the modified Bessel function of the first kind (see Appendix A). From these exact expressions, we can readily obtain the asymptotics of the magnetoresistance (8) in high carrier-density region as follows; For $|n| \gg 1$,

$$\Delta\rho(n,\theta,B_{\parallel}) \simeq \begin{cases} \frac{1}{2} (\sin^2\theta + 3\cos^2\theta) \frac{(ZB_{\parallel})^2}{\sqrt{\pi}\hbar R} |n|^{-3/2} \log(R|n|^{1/2}), & \text{for exponential (i)} \\ \frac{1}{4} (\sin^2\theta + 3\cos^2\theta) \frac{(ZB_{\parallel})^2}{\hbar R} |n|^{-3/2}, & \text{for Gaussian (ii)}. \end{cases}$$
(11)

The asymptotic for the Gaussian case (ii) shown in the second line in (11) is exactly the same as Eq.(3) reported in [17]. On the other hand, there is a logarithmic correction to the $|n|^{-3/2}$ -law in the case (i) with the exponential height-correlation of ripples.

For the low carrier-density region, we have found the following behavior for the magnetoresistance; when $|n| \simeq 0$,

$$\Delta\rho(n,\theta,B_{\parallel}) \simeq \begin{cases} \frac{1}{2}(\sin^2\theta + 3\cos^2\theta) \frac{(\pi ZRB_{\parallel})^2}{\hbar} \left(1 - \frac{9}{2}\pi R^2|n|\right), & \text{for exponential (i)} \\ \frac{1}{4}(\sin^2\theta + 3\cos^2\theta) \frac{(\pi ZRB_{\parallel})^2}{\hbar} \left(1 - \frac{3}{4}\pi R^2|n|\right), & \text{for Gaussian (ii)}. \end{cases}$$
(12)

That is, $\rho(n, \theta, B_{\parallel})$ shows a cusp at the charge neutrality point |n| = 0 and the dependence on n around this point is linear $\propto -|n|$. In the vicinity of charge neutrality point, electronic transport will be affected by strong density inhomogeneity in rippled graphene, which is called electron-hole puddle [4]. Moreover, in low carrier-density region, $|n| \ll 1$, we have $kR \ll 1$ and the semi-classical Boltzmann transport theory is afraid to be broken-down. In order to give 'the 0-th order approximation', to which corrections by more elaborate approximations or full quantum theory will be added [4], however, here we try to apply our analytic results to the experimental data in the whole region of n. The result seems to be excellent if we assume the Gaussian height-correlation of ripples. See Figures 2 and 3 in Section IV.

The paper is organized as follows. In Section II we give a derivation of the Lundeberg-Folk formula (8) from a semi-classical model using the Boltzmann transport theory. Section III is devoted to the proofs of our exact expressions (9) and (10) and their asymptotics (11) and (12). In Section IV, we discuss comparison of the present analytic results with the

experimental data measured by Wakabayashi and his coworkers. Appendix A is prepared for giving the mathematical formulas for special functions used in the text. In Appendix B an explanation is given for the linear relation between resistance and inverse of relaxation time based on the Boltzmann transport theory.

II. DERIVATION OF LUNDEBERG-FOLK FORMULA

As remarked just below Eq.(8), the general expression of $\Delta \rho$ as a functional of the height-correlation function c(r) of ripples, (8) with (5) and (6), is found only in [18]. Although the essence of its derivation is given there, the description is very brief. For convenience, here we would like to complete the derivation of the Lundeberg-Folk formula (8) following [18].

We take the averaged 2D plane of graphene as the x-y plane. Let $h(\mathbf{r})$ be the height of ripple at $\mathbf{r} = (x, y)$.

A. Geometric vector potential

Under the in-plane magnetic field in the x-direction,

$$\boldsymbol{B}_{\parallel} = (B_{\parallel}, 0), \tag{13}$$

the geometric vector potential of Berry [24], $\mathbf{A}(\mathbf{r}) = (A_x(\mathbf{r}), A_y(\mathbf{r}))$, is calculated as [25]

$$A_x(\mathbf{r}) = 0, \qquad A_y(\mathbf{r}) = -B_{\parallel}h(\mathbf{r}).$$
 (14)

It gives a potential expressed by a 2×2 complex matrix for Dirac fermions with electric charge -e and the Fermi velocity $v_{\rm F}$,

$$U(\mathbf{r}) = -ev_{F}\mathbf{A}(\mathbf{r}) \cdot \boldsymbol{\sigma}$$

$$= ev_{F}B_{\parallel}h(\mathbf{r})\sigma_{y}$$

$$= ev_{F}B_{\parallel}h(\mathbf{r})\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad (15)$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ are Pauli matrices.

B. Scattering matrix

The scattering matrix for an interaction operator \mathcal{U} is calculated by the Fermi golden rule as

$$S_{\text{ripple}}(\mathbf{k}, \mathbf{k}') = \frac{2\pi V}{\hbar} |\langle \mathbf{k}' | \mathcal{U} | \mathbf{k} \rangle|^2 \delta(E(k') - E(k))$$

$$= \frac{2\pi V}{\hbar^2 v_F} |\langle \mathbf{k}' | \mathcal{U} | \mathbf{k} \rangle|^2 \delta(k' - k), \qquad (16)$$

where $E(k) = \hbar v_{\rm F} k$. We note that

$$\langle \mathbf{k}' | \mathcal{U} | \mathbf{k} \rangle = \int d^2 r' \int d^2 r \, \langle \mathbf{k}' | \mathbf{r}' \rangle \langle \mathbf{r}' | \mathcal{U} | \mathbf{r} \rangle \langle \mathbf{r} | \mathbf{k} \rangle \tag{17}$$

with

$$\langle \mathbf{r}' | \mathcal{U} | \mathbf{r} \rangle = U(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}'),$$
 (18)

where the potential $U(\mathbf{r})$ is given by (15), $\delta(\mathbf{r}-\mathbf{r}') = \delta(x-x')\delta(y-y')$, and $\langle \mathbf{k}'|\mathbf{r}\rangle = \langle \mathbf{r}'|\mathbf{k}'\rangle^{\dagger}$. By using the two-component plane wave solution (2) for $E = E_+ = \hbar v_{\rm F} k$, (17) becomes

$$\langle \mathbf{k}' | \mathcal{U} | \mathbf{k} \rangle = \int d^{2}r \frac{e^{-i\mathbf{k}' \cdot \mathbf{r}}}{\sqrt{2V}} (e^{i\theta_{k'}/2} e^{-i\theta_{k'}/2}) \left\{ ev_{F} B_{\parallel} h(\mathbf{r}) \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \right\} \frac{e^{i\mathbf{k} \cdot \mathbf{r}}}{\sqrt{2V}} \begin{pmatrix} e^{-i\theta_{k}/2} \\ e^{i\theta_{k}/2} \end{pmatrix}$$

$$= \frac{ev_{F} B_{\parallel}}{V} \sin \frac{\theta_{k} + \theta_{k'}}{2} \hat{h}^{*}(\mathbf{q})$$
(19)

with q = k' - k and

$$\widehat{h}^*(\boldsymbol{q}) = \int d^2r \, e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} h(\boldsymbol{r}). \tag{20}$$

The square of (20), $|\widehat{h}(\boldsymbol{q})|^2 = \widehat{h}(\boldsymbol{q})\widehat{h}^*(\boldsymbol{q})$, is then calculated as

$$|\widehat{h}(\boldsymbol{q})|^{2} = \int d^{2}r \int d^{2}r' e^{i\boldsymbol{q}\cdot(\boldsymbol{r}'-\boldsymbol{r})}h(\boldsymbol{r})h(\boldsymbol{r}')$$

$$= V \int d^{2}r e^{i\boldsymbol{q}\cdot\boldsymbol{r}} \frac{1}{V} \int d^{2}r_{0} h(\boldsymbol{r}_{0})h(\boldsymbol{r}_{0}+\boldsymbol{r}), \qquad (21)$$

where we have renamed the integration variable as $\mathbf{r} \to \mathbf{r}_0$ and $\mathbf{r}' - \mathbf{r} \to \mathbf{r}$. The quantity involving the second integral in the second line of (21), $(1/V) \int d^2r_0h(\mathbf{r}_0)h(\mathbf{r}_0 + \mathbf{r})$, is a volume average of a product $h(\mathbf{r}_0)h(\mathbf{r}_0 + \mathbf{r})$ with respect to \mathbf{r}_0 over the system. If the distribution of the ripple height $h(\mathbf{r})$ on graphene is translation invariant, this volume average will converge to the height correlation function (4) as $V \to \infty$, by the self-averaging property

of usual random systems. Moreover, it can be written as c(r), if the system is also isotropic. Therefore, provided that V is large enough, (21) is equal to the Fourier transform of c(r)

$$\widehat{c}(q) = \int d^2 r \, e^{i\boldsymbol{q}\cdot\boldsymbol{r}} c(r), \quad q = |\boldsymbol{q}| \tag{22}$$

multiplied by the volume V of the system; $|\widehat{h}(\boldsymbol{q})|^2 = V\widehat{c}(q)$. Inserting the above results into (16), the volume factor V is cancelled out as desired, and we obtain the following expression of scattering matrix,

$$S_{\text{ripple}}(\mathbf{k}, \mathbf{k}') = \frac{2\pi e^2 v_F B_{\parallel}^2}{\hbar^2} \sin^2 \frac{\theta_k + \theta_{k'}}{2} \widehat{c}(q) \delta(k' - k), \quad \mathbf{q} = \mathbf{k}' - \mathbf{k}, \quad q = |\mathbf{q}|,$$
 (23)

which was given as Eq.(A.1) in [18].

By definition of θ_k for $\mathbf{k} = (k_x, k_y)$ given by (3) and its analogue $\theta_{k'}$ for $\mathbf{k'} = (k'_x, k'_y)$, under the energy conservation k' = k, $q_x = k'_x - k_x = k(\cos \theta_{k'} - \cos \theta_k)$, $q_y = k'_y - k_y = k(\sin \theta_{k'} - \sin \theta_k)$, and thus

$$q = |\mathbf{q}| = \sqrt{q_x^2 + q_y^2}$$

$$= 2k\sqrt{1 - \cos(\theta_k - \theta_{k'})}$$

$$= 2k\sin\frac{\theta_k - \theta_{k'}}{2}.$$
(24)

Then, when $\mathbf{q} = \mathbf{k}' - \mathbf{k}$ with the condition k' = k, (22) becomes

$$\widehat{c}(q) = \int_0^\infty dr \, r \int_0^{2\pi} d\varphi \, c(r) e^{iqr \cos \varphi}$$

$$= \int_0^\infty dr \, r c(r) \int_0^{2\pi} d\varphi \exp \left[2ikr \sin \frac{\theta_k - \theta_{k'}}{2} \cos \varphi \right]. \tag{25}$$

C. Boltzmann equation and scattering rates

Lundeberg and Folk introduced a semi-classical model based on the Boltzmann transport theory for the system, in which the 2D electronic state with a wave-number vector \mathbf{k} is described by probability distribution $f(\mathbf{k})$. The time evolution of $f(\mathbf{k})$ follows the Boltzmann equation (see, for example, [26, 27])

$$\left(\frac{\partial}{\partial t} + \frac{e}{\hbar} \mathbf{E} \cdot \nabla_k\right) f(\mathbf{k}) = \left[\frac{\partial f(\mathbf{k})}{\partial t}\right]_{S},\tag{26}$$

in the external electric field E, where we have assumed the spatial homogeneity of distribution f and omitted the term $\mathbf{v} \cdot \nabla_r f(\mathbf{k})$ in the LHS. The 'collision term' in the RHS, which describes the scattering of particles or holes by random vector potentials caused by ripples in the present system, is given by

$$\left[\frac{\partial f(\mathbf{k})}{\partial t}\right]_{S} = D[S, f](\mathbf{k}) \tag{27}$$

with the operator

$$D[S, f](\mathbf{k}) = \int \frac{d^2k'}{(2\pi)^2} S(\mathbf{k}, \mathbf{k}') \Big[f(\mathbf{k}') - f(\mathbf{k}) \Big]$$
(28)

where $S = S_0 + S_{\text{ripple}}$ is the total scattering matrix. Here S_0 is the zero field scattering matrix assumed to be in the isotropic form, $S_0(\mathbf{k}, \mathbf{k}') = s_0(k, q)\delta(k - k')$, and S_{ripple} is given by (23). We set $S(\mathbf{k}, \mathbf{k}') = \widetilde{S}(\mathbf{k}, \mathbf{k}')\delta(k - k')$ and rewrite (28) as

$$D[S, f](\mathbf{k}) = \frac{k}{(2\pi)^2} \int_{-\pi}^{\pi} d\theta_{k'} \widetilde{S}(\mathbf{k}, \mathbf{k}') \left[\widetilde{f}(\theta_{k'}) - \widetilde{f}(\theta_k) \right], \tag{29}$$

where $\widetilde{f}(\theta_k)$ shows the dependence of $f(\mathbf{k})$ on the angular component θ_k of \mathbf{k} , when $k = |\mathbf{k}|$ is given. In order to study θ_k -dependence of scattering induced by \mathbf{B}_{\parallel} , which is imposed in the x-direction, we introduce the following orthogonal bases,

$$\widetilde{f}_x(\theta_k) = \frac{\cos \theta_k}{\sqrt{\pi}}, \quad \widetilde{f}_y(\theta_k) = \frac{\sin \theta_k}{\sqrt{\pi}},$$
(30)

satisfying

$$\int_{-\pi}^{\pi} d\theta_k \, \widetilde{f}_{\alpha}(\theta_k) \widetilde{f}_{\beta}(\theta_k) = \delta_{\alpha,\beta}, \qquad \alpha, \beta = x, y.$$
(31)

The B_{\parallel} -induced parts of scattering rates, which give the inverses of transport times enhanced by B_{\parallel} , are obtained as

$$\Delta \tau_{\alpha,\beta}^{-1}(k) = -\int_{-\pi}^{\pi} d\theta_k \, \widetilde{f}_{\alpha}(\theta_k) D[\widetilde{S}_{\text{ripple}}, \widetilde{f}_{\beta}](\theta_k)$$
 (32)

for $\alpha, \beta = x, y$, by the orthogonality relation (31) of the two bases (30).

Now combining (32) and (29) with (23) and (25), we have multiple-integral expressions for $\Delta \tau_{\alpha,\beta}^{-1}$ such that integrals are performed with respect to $\theta_k, \theta_{k'}, r$ and φ . Change the integral variables as $\theta_k + \theta_{k'} \to \theta_+$, $\theta_k - \theta_{k'} \to \theta_-$, and let

$$L_{\alpha,\beta}(k,r,\theta_{-}) = \int_{0}^{4\pi} d\theta_{+} \int_{0}^{2\pi} d\varphi \exp\left[2ikr\sin\frac{\theta_{-}}{2}\cos\varphi\right] \sin^{2}\frac{\theta_{+}}{2}$$
$$\times \widetilde{f}_{\alpha}\left(\frac{\theta_{+}+\theta_{-}}{2}\right) \left[\widetilde{f}_{\beta}\left(\frac{\theta_{+}-\theta_{-}}{2}\right) - \widetilde{f}_{\beta}\left(\frac{\theta_{+}+\theta_{-}}{2}\right)\right], \tag{33}$$

 $\alpha, \beta = x, y$. Then

$$\Delta \tau_{\alpha,\beta}^{-1}(k) = -\frac{e^2 v_{\rm F} B_{\parallel}^2}{4\pi\hbar^2} k \int_0^{\infty} dr \, r c(r) \int_0^{2\pi} d\theta_- L_{\alpha,\beta}(k,r,\theta_-), \quad \alpha,\beta = x, y.$$
 (34)

By the Boltzmann transport theory (see Appendix B for an explanation), the resistances induced by $\boldsymbol{B}_{\parallel}$ are related with $\tau_{\alpha,\beta}^{-1}$ as

$$\Delta \rho_{\alpha,\beta}(k) = \frac{2\pi\hbar}{e^2 v_{\rm F} k} \Delta \tau_{\alpha,\beta}^{-1}(k), \quad \alpha, \beta = x, y.$$
 (35)

We performed the integrals (33) and obtained the results

$$L_{xx}(k, r, \theta_{-}) = 3L_{yy}(k, r, \theta_{-}) = -3\pi J_0 \left(2kr\sin\frac{\theta_{-}}{2}\right)\sin^2\frac{\theta_{-}}{2},$$
 (36)

$$L_{xy}(k, r, \theta_{-}) = -\frac{1}{3}L_{yx}(k, r, \theta_{-}) = -\pi J_0\left(2kr\sin\frac{\theta_{-}}{2}\right)\sin\theta_{-},$$
 (37)

where $J_0(z)$ is the Bessel function with index $\nu = 0$ (see Appendix A).

Then (35) with (34) gives

$$\Delta \rho_{xx}(k) = 3\Delta \rho_{yy}(k) = \frac{3\pi B_{\parallel}^2}{2\hbar} g(k), \tag{38}$$

$$\Delta \rho_{xy}(k) = \Delta \rho_{yx}(k) = 0, \tag{39}$$

where g(k) is given by (5) with (6). The 'threefold relation' between $\Delta \rho_{xx}$ and $\Delta \rho_{yy}$ is found in (38) [17, 18, 28].

D. Lundeberg-Folk formula

Let $\mathbf{E} = (E_x, E_y)$ be the in-plane electric field applied in order to measure resistance. If the current is written as $\mathbf{J} = (J_x, J_y)$, then the resistance coefficients $\Delta \rho_{\alpha,\beta}$, $\alpha, \beta = x, y$, are defined as

$$\begin{pmatrix} E_x \\ E_y \end{pmatrix} = \begin{pmatrix} \Delta \rho_{xx} & \Delta \rho_{xy} \\ \Delta \rho_{yx} & \Delta \rho_{yy} \end{pmatrix} \begin{pmatrix} J_x \\ J_y \end{pmatrix}. \tag{40}$$

In the isotropic system, $\Delta \rho_{xy} = \Delta \rho_{yx} = 0$ as in (39), then $E_x = \Delta \rho_{xx} J_x$, $E_y = \Delta \rho_{yy} J_y$. We have chosen the direction of \mathbf{B}_{\parallel} in the x-direction as (13). Then, if we denote the angle between \mathbf{B}_{\parallel} and \mathbf{J} as θ , $J_x = J\cos\theta$, $J_y = J\sin\theta$ with $J = |\mathbf{J}|$ and the \mathbf{B}_{\parallel} -induced resistance $\Delta \rho$ for the current \mathbf{J} is given by

$$\Delta \rho = \frac{\boldsymbol{E} \cdot \boldsymbol{J}}{J^2}$$

$$= \frac{1}{J^2} (\Delta \rho_{xx} J_x^2 + \Delta \rho_{yy} J_y^2)$$

$$= \Delta \rho_{xx} \cos^2 \theta + \Delta \rho_{yy} \sin^2 \theta. \tag{41}$$

Then by the threefold relation (38) between $\Delta \rho_{xx}$ and $\Delta \rho_{yy}$, the Lundeberg-Folk formula (8) is obtained.

III. PROOFS OF RESULTS

A. Proof of Eq.(9)

Let $c(r) = Z^2 e^{-r/R}$ and use the formula (A3) for $\nu = 0$. Then (5) with (6) is written as

$$g(k) = Z^2 \sum_{n=0}^{\infty} \frac{(-k^2)^n}{(n!)^2} M_r(n) M_{\phi}(n)$$
(42)

with

$$M_r(n) = \int_0^\infty dr \, r^{2n+1} e^{-r/R} = R^{2n+2} \Gamma(2n+2),$$

$$M_\phi(n) = \int_0^{2\pi} d\phi \, \sin^{2n+2} \frac{\phi}{2} = \frac{2\sqrt{\pi} \Gamma(n+3/2)}{\Gamma(n+2)}.$$
(43)

We apply the duplication formula (A2) of Gamma functions and use the Pochhammer symbol (A5), then we have

$$g(k) = (ZR)^{2} \sum_{n=0}^{\infty} \frac{\{2\Gamma(n+3/2)\}^{2}}{n!\Gamma(n+2)} (-(2kR)^{2})^{n}$$

$$= \pi (ZR)^{2} \sum_{n=0}^{\infty} \frac{\{(3/2)_{n}\}^{2}}{(2)_{n}} \frac{(-(2kR)^{2})^{n}}{n!},$$
(44)

which prove the first equality of (9) by the definition of the Gauss hypergeometric function (A6).

From the recurrence relations (A8) and (A9), we obtain the following two equalities,

$$F\left(\frac{3}{2}, \frac{3}{2}, 2; -(2kR)^2\right) = \frac{1}{2(kR)^2} \left[F\left(\frac{1}{2}, \frac{1}{2}, 1; -(2kR)^2\right) - F\left(\frac{1}{2}, \frac{3}{2}, 1; -(2kR)^2\right) \right],$$

$$F\left(\frac{1}{2}, \frac{3}{2}, 1; -(2kR)^2\right) = \frac{1}{1 + (2kR)^2} F\left(-\frac{1}{2}, \frac{1}{2}, 1; -(2kR)^2\right). \tag{45}$$

Combining them gives

$$F\left(\frac{3}{2}, \frac{3}{2}, 2; -(2kR)^{2}\right)$$

$$= \frac{1}{2(kR)^{2}} \left[F\left(\frac{1}{2}, \frac{1}{2}, 1; -(2kR)^{2}\right) - \frac{1}{1 + (2kR)^{2}} F\left(-\frac{1}{2}, \frac{1}{2}, 1; -(2kR)^{2}\right) \right]. \quad (46)$$

By the formulas (A14), which express the complete elliptic integrals K(z) and E(z) by using the Gauss hypergeometric functions, the second equality of (9) is proved.

B. Proof of Eq.(10)

Let $c(r) = Z^2 e^{-(r/R)^2}$ and use the formula (A3) for $\nu = 0$. Then (5) with (6) is written as

$$g(k) = Z^2 \sum_{n=0}^{\infty} \frac{(-k^2)^n}{(n!)^2} \widetilde{M}_r(n) M_{\phi}(n), \tag{47}$$

where

$$\widetilde{M}_r(n) = \int_0^\infty dr \, r^{2n+1} e^{-r^2/R^2} = \frac{1}{2} R^{2n+2} n!$$
 (48)

and $M_{\phi}(n)$ is given as in (43). Following the similar procedure mentioned above, we have

$$g(k) = \frac{\pi (ZR)^2}{2} \sum_{n=0}^{\infty} \frac{(3/2)_n}{(2)_n} \frac{(-(kR)^2)^n}{n!},$$
(49)

which proves the first equality of (10) by the definition of the confluent hypergeometric function (A7).

From the recurrence relations (A10) and (A11), we obtain the following equality,

$$F(\alpha+1,\gamma;z) = F(\alpha,\gamma-1;z) + \frac{z(\alpha-\gamma+1)}{\gamma(1-\gamma)}F(\alpha+1,\gamma+1;z).$$
 (50)

By using this equality for $\alpha = 1/2$ and $\gamma = 2$, we can rewrite the first line of (10) as

$$g(k) = \frac{\pi (ZR)^2}{2} \left[F\left(\frac{1}{2}, 1; -(kR)^2\right) - \frac{(kR)^2}{4} F\left(\frac{3}{2}, 3; -(kR)^2\right) \right]. \tag{51}$$

By the formula (A15), which expresses the modified Bessel function $I_{\nu}(z)$ by using the confluent hypergeometric functions, the second equality of (10) is proved.

C. Asymptotics in high carrier-density region

Case (i): the exponential height-correlation

In Gauss' integral representation (A12), if we change the variable as $u = (w-1)/(4(kR)^2)$, we have

$$F\left(\frac{3}{2}, \frac{3}{2}, 2; -(2kR)^2\right) = \frac{1}{4\pi (kR)^3} \int_1^{1+4(kR)^2} dw (w-1)^{1/2} \left(1 - \frac{w-1}{4(kR)^2}\right)^{-1/2} w^{-3/2}.$$
 (52)

Then we obtain the equality

$$F\left(\frac{3}{2}, \frac{3}{2}, 2; -(2kR)^{2}\right)$$

$$= \frac{1}{\pi (kR)^{3}} \left(4 + \frac{1}{(kR)^{2}}\right)^{-1/2} \left[K\left(\sqrt{\frac{(2kR)^{2}}{1 + (2kR)^{2}}}\right) - E\left(\sqrt{\frac{(2kR)^{2}}{1 + (2kR)^{2}}}\right)\right]. \tag{53}$$

By the asymptotics of the complete elliptic integrals [29]

$$K(z) \simeq \log\left(\frac{4}{\sqrt{1-z^2}}\right),$$

 $E(z) \simeq 1, \quad \text{as } z \to 1,$ (54)

we have the behavior

$$F\left(\frac{3}{2}, \frac{3}{2}, 2; -(2kR)^2\right) \simeq \frac{1}{\pi (kR)^2} \left[\log(4\sqrt{1 + (2kR)^2}) - 1\right], \text{ as } k \to \infty.$$
 (55)

Through the relation (7) between k and n, the Lundeberg-Folk formula (8) with the present result (9) gives the first line of the RHS of (11).

Case (ii): the Gaussian height-correlation

In this case, we use the asymptotic expansion formula of the confluent hypergeometric function,

$$F(\alpha, \gamma; z) \simeq \frac{\Gamma(\gamma)}{\Gamma(\gamma - \alpha)} (-z)^{-\alpha} \sum_{n=0}^{\infty} (-1)^n \frac{(\alpha)_n (\gamma - \alpha)_n}{n!} z^{-n} + \frac{\Gamma(\gamma)}{\Gamma(\alpha)} e^z z^{\alpha - \gamma} \sum_{n=0}^{\infty} \frac{(1 - \alpha)_n (\gamma - \alpha)_n}{n!} z^{-n}.$$
 (56)

It gives

$$F\left(\frac{3}{2}, 2; -(kR)^2\right) \simeq \frac{1}{\sqrt{\pi}(kR)^3} + \mathcal{O}((kR)^{-5}),$$
 (57)

and we obtain the second line of the RHS of (11). This result is exactly the same as Eq.(3) reported in [17].

D. Behavior in low carrier-density region

Case (i): the exponential height-correlation

By using the first two terms of the series (A6) defining the Gauss hypergeometric function, we obtain from (9)

$$g(k) = \pi (ZR)^2 \left[1 - \frac{9}{2} (kR)^2 + \mathcal{O}((kR)^4) \right].$$
 (58)

The first line of the RHS of (12) is concluded from (58).

Case (ii): the Gaussian height-correlation

By using the first two terms of the series (A7) defining the confluent hypergeometric function, we obtain from (10)

$$g(k) = \frac{\pi (ZR)^2}{2} \left[1 - \frac{3}{4} (kR)^2 + \mathcal{O}((kR)^4) \right].$$
 (59)

It gives the second line of the RHS of (12).

IV. CONCLUDING REMARKS

The Lundeberg-Folk formula (8) shows that the magnetoresistance induced by $\boldsymbol{B}_{\parallel}$ is proportional to $B_{\parallel}^2,$

$$\Delta \rho(n, \theta, B_{\parallel}) = a(n, \theta) B_{\parallel}^2. \tag{60}$$

The coefficient $a(n, \theta)$ is given by

$$a(n,\theta) = \frac{\pi}{2\hbar} (\sin^2 \theta + 3\cos^2 \theta) g(\sqrt{\pi |n|}), \tag{61}$$

in which the function g depends on the height-correlation function c(r) of ripples on graphene. In the present paper, we have clarified the dependence of $\Delta \rho$ on c(r) for the two cases, (i) $c(r) = Z^2 e^{-r/R}$ (exponential) and (ii) $c(r) = Z^2 e^{-(r/R)^2}$ (Gaussian), where $Z^2 = c(0) = \langle h^2 \rangle$ is the variance of height of ripples and R indicates the correlation length of ripples.

In the low carrier-density region, the so-called electron-hole puddles appear on the rippled graphene and the homogeneity assumption of system will be invalid. In order to handle the inhomogeneity of the carrier density around the Dirac point, the present Boltzmann approach should be corrected including higher-level approximations [4, 30, 31]. Away from the charge neutrality point, however, the semi-classical modeling based on the Boltzmann transport theory works well to describe the electronic transport properties of graphene. Here we consider our analytic expressions for $\Delta \rho$ as 'trial interpolation formulas' connecting two high-carrier-density regimes, $|n| \gg 1$; the positive-charge regime (n > 0) and the negative one (n < 0).

Our expressions for $\Delta \rho$ reported in this paper include two parameters Z and R. If experimental data are provided, we can evaluate the standard deviation of ripple height $Z = \sqrt{\langle h^2 \rangle}$ and the correlation length of ripples R by numerical fitting of the data to our analytic expressions (9) or (10).

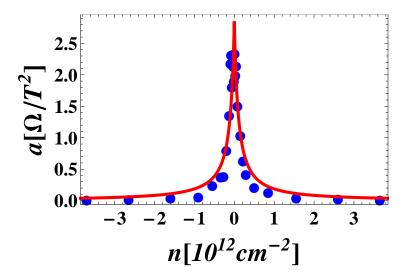


FIG. 1: The coefficient $a(n, \theta)$ of the Lundeberg-Folk formula (61) for $\theta = 0$ with the present exact solution (9) for the exponential height-correlation of ripples is drawn. The parameters are chosen as Z = 0.531 [nm] and R = 8.51 [nm] by the best fitting to the experimental data given by Wakabayashi and his coworkers (indicated by dots).

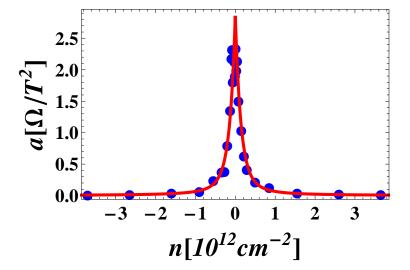


FIG. 2: The coefficient $a(n,\theta)$ of the Lundeberg-Folk formula (61) for $\theta=0$ with the present exact solution (10) for the Gaussian height-correlation of ripples is drawn. The parameters are chosen as Z=0.376 [nm] and R=17.0 [nm] by the best fitting to the experimental data given by Wakabayashi and his coworkers (indicated by dots). The curve fits the experimental data very well in the whole region of carrier-density n.

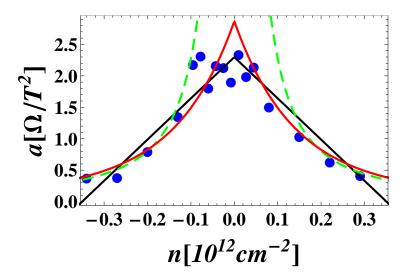


FIG. 3: Enlarged figure of Fig.2 in the vicinity of the charge neutrality point (|n| = 0). Dots are the experimental data given by Wakabayashi and his coworkers. The bold curve showing a cusp at |n| = 0 is the present analytic solution (10) for the Gaussian height-correlation with Z = 0.376 [nm] and R = 17.0 [nm]. In this low carrier-density region, the $|n|^{-3/2}$ -law shown by dotted curves is invalid, since it diverges as $|n| \to 0$. In the very vicinity of the point |n| = 0, the simple expression given in the second line of the RHS of (12) will work well, which is shown by thin black lines.

Figures 1 and 2 show results of numerical fitting of the Lundeberg-Folk formula (8) with our exact solutions (9) and (10) for the exponential and the Gaussian height-correlations to the experimental data, respectively, when $\theta = 0$ in the both cases. The experimental data are given by Wakabayashi and his coworkers [19, 20]. As we can see in these figures, the fitting in the high carrier-density region is more excellent in the Gaussian case (Fig.2) than in the exponential case (Fig.1).

For the vicinity of the charge neutrality point, $|n| \simeq 0$, the fitting result for the Gaussian height-correlation is shown by Fig. 3, in which the $|n|^{-3/2}$ -law for the high carrier-density region $|n| \gg 1$ (the second line of (11)) and the expression for $|n| \simeq 0$ (the second line of (12)) are also plotted for comparison. The obtained values of parameters by the present numerical fitting are Z=0.376 [nm] and R=17.0 [nm], respectively. These values should be compared with the direct experimental measurements [7, 12, 17, 19, 20]. In particular, it was reported in [20] the AFM measurements gave Z=0.118 [nm] and R=15.2 [nm]. See also experimental values cited in [17, 18] from [7, 12] and others. (We note that recent high-resolution measurements and analysis have revealed smaller-sized roughness of the substrate

and graphene surfaces [32].)

We hope that the our expressions will be used for systematic analysis of experimental data also for different values of θ . In the present paper, we have assumed translation invariance and isotropy for distribution of ripple height. Even in the high carrier-density regions, apart from the effect of electron-hole puddles, further calculation for general setting of ripple-height-correlations will be an interesting future problem.

Acknowledgments

The present authors would like to thank Junichi Wakabayashi for providing them experimental data of magnetoresistance measurements and for very useful discussion on the present work. They also thank Tohru Kawarabayashi and Mark Lundeberg for helpful comments on the present study. This work is supported in part by the Grant-in-Aid for Scientific Research (C) (No.21540397) of Japan Society for the Promotion of Science.

Appendix A: Definitions and formulas of special functions

Here we list the definitions and formulas of special functions used in the text (see, for instance, [22]). The gamma function $\Gamma(z)$ is defined by

$$\Gamma(z) = \int_0^\infty e^{-u} u^{z-1} du, \quad \Re z > 0.$$
 (A1)

When $n \in \mathbb{N}_0 \equiv \{0, 1, 2, \dots\}$, $\Gamma(n+1) = n!$ (we set $0! \equiv 1$). The following equality is called the duplication formula,

$$\Gamma(2z) = \frac{2^{2z}}{2\sqrt{\pi}}\Gamma(z)\Gamma(z+1/2). \tag{A2}$$

The Bessel function $J_{\nu}(z)$ with index $\nu \in \mathbb{R}$ is given by

$$J_{\nu}(z) = \left(\frac{z}{2}\right)^{\nu} \sum_{n=0}^{\infty} \frac{(-1)^n (z/2)^{2n}}{n!\Gamma(\nu+n+1)}$$
(A3)

for a complex number z which is not negative real. Then the modified Bessel function of the first kind is defined as

$$I_{\nu}(z) = \begin{cases} e^{-\nu\pi i/2} J_{\nu}(ze^{\pi i/2}) & (-\pi < \arg z \le \pi/2) \\ e^{3\nu\pi i/2} J_{\nu}(ze^{-3\pi i/2}) & (\pi/2 < \arg z \le \pi) \end{cases}$$
$$= \left(\frac{z}{2}\right)^{\nu} \sum_{n=0}^{\infty} \frac{(z/2)^{2n}}{n!\Gamma(\nu+n+1)}. \tag{A4}$$

For $n \in \mathbb{N}_0$, the Pochhammer symbol is defined as

$$(\alpha)_n = \alpha(\alpha+1)(\alpha+2)\cdots(\alpha+n-1), \quad n \in \mathbb{N} \equiv \{1, 2, 3, \dots\},$$

$$(\alpha)_0 = 1.$$
(A5)

The Gauss hypergeometric function is defined by

$$F(\alpha, \beta, \gamma; z) = \sum_{n=0}^{\infty} \frac{(\alpha)_n (\beta)_n}{(\gamma)_n} \frac{z^n}{n!},$$
(A6)

and the confluent hypergeometric function is defined as

$$F(\alpha, \gamma; z) = \lim_{\beta \to \infty} F(\alpha, \beta, \gamma; z/\beta)$$

$$= \sum_{n=0}^{\infty} \frac{(\alpha)_n}{(\gamma)_n} \frac{z^n}{n!}.$$
(A7)

The following recurrence relations for $F(\alpha, \beta, \gamma; z)$ are known,

$$\gamma[F(\alpha, \beta + 1, \gamma; z) - F(\alpha, \beta, \gamma; z)] = \alpha z F(\alpha + 1, \beta + 1, \gamma + 1; z), \tag{A8}$$

$$\alpha(1-z)F(\alpha+1,\beta,\gamma;z) + [\gamma - 2\alpha + (\alpha-\beta)z]F(\alpha,\beta,\gamma;z)$$

$$+(\alpha - \gamma)F(\alpha - 1, \beta, \gamma; z) = 0.$$
 (A9)

For $F(\alpha, \beta; z)$,

$$zF(\alpha+1,\gamma+1;z) = \gamma[F(\alpha+1,\gamma;z) - F(\alpha,\gamma;z)],\tag{A10}$$

$$\alpha F(\alpha + 1, \gamma + 1; z) = (\alpha - \gamma) F(\alpha, \gamma + 1; z) + \gamma F(\alpha, \gamma; z) \tag{A11}$$

are satisfied. The Gauss hypergeometric function has the following integral expression,

$$F(\alpha, \beta, \gamma; z) = \frac{\Gamma(\gamma)}{\Gamma(\beta)\Gamma(\gamma - \beta)} \int_0^1 du \, u^{\beta - 1} (1 - u)^{\gamma - \beta - 1} (1 - uz)^{-\alpha}. \tag{A12}$$

The complete elliptic integrals of the first kind, K(z), and of the second kind, E(z), are defined as

$$K(z) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1 - z^2 \sin^2 \theta}} = \int_0^1 \frac{du}{\sqrt{(1 - u^2)(1 - z^2 u^2)}},$$

$$E(z) = \int_0^{\pi/2} \sqrt{1 - z^2 \sin^2 \theta} d\theta,$$
(A13)

respectively. They are expressed by using the Gauss hypergeometric functions as

$$K(z) = \frac{\pi}{2} F\left(\frac{1}{2}, \frac{1}{2}, 1; z^2\right), \quad E(z) = \frac{\pi}{2} F\left(-\frac{1}{2}, \frac{1}{2}, 1; z^2\right).$$
 (A14)

The modified Bessel function (A4) is expressed by using the confluent hypergeometric functions as

$$I_{\nu}(z) = \frac{(z/2)^{\nu}}{\Gamma(\nu+1)} e^{z} F\left(\nu + \frac{1}{2}, 2\nu + 1; -2z\right). \tag{A15}$$

Appendix B: Linear relation between ρ and τ^{-1}

Let $f_0(k) = [e^{(E(k)-\mu)/(k_BT)} + 1]^{-1}$ be the equilibrium Fermi distribution function at temperature T and chemical potential μ . The relaxation time $\tau(k)$ is phenomenologically introduced as

$$\left[\frac{\partial f(k)}{\partial t}\right]_{S} = -\frac{\delta f(k)}{\tau(k)} \quad \text{with} \quad \delta f(k) = f(k) - f_0(k). \tag{B1}$$

When we consider the long-term limit, $\partial f(k)/\partial t$ -term in the LHS is zero, and we have

$$\delta f(k) = -\frac{e}{\hbar} \tau(k) \mathbf{E} \cdot \nabla_k f(k)$$

$$\simeq -\frac{e}{\hbar} \tau(k) \mathbf{E} \cdot \nabla_k f_0(k). \tag{B2}$$

In low temperature limit, $E = \hbar v_F k$ and $\mathbf{E} \cdot \nabla_k f_0(k) \simeq \hbar v_F |\mathbf{E}| \partial f_0(k) / \partial E \simeq |\mathbf{E}| \delta(k - k_F)$, where k_F denotes the Fermi wave-number. Then in the 2D plane the current is calculated as follows, provided \mathbf{J} and \mathbf{E} are parallel;

$$J = |\mathbf{J}| = \int \frac{d^2k}{(2\pi)^2} (-ev_{\rm F}) \delta f(k)$$

$$\simeq \int_0^\infty \frac{dk}{2\pi} k(-ev_{\rm F}) \left(-\frac{e}{\hbar} \tau(k) |\mathbf{E}| \delta(k - k_{\rm F}) \right)$$

$$= \frac{e^2 v_{\rm F} k_{\rm F} \tau(k_{\rm F})}{2\pi \hbar} |\mathbf{E}|. \tag{B3}$$

Since resistance ρ is defined as $J = \rho^{-1} |\mathbf{E}|$, we have the linear relation between ρ and τ^{-1} as $\rho = c\tau^{-1}$ with the coefficient $c = 2\pi\hbar/(e^2v_{\rm F}k_{\rm F})$. In Eq.(35) $k_{\rm F}$ is written as k.

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